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=> d que l70
L13              STR
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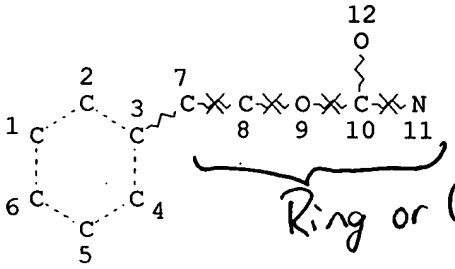


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CONNECT IS E1  RC AT  12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   3
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L26         616 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND NRS<2 AND NR<2
L65          40 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND 46.220/RID
L68         744 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND NRS<3 AND NR<3 AND
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L70          17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L65 OR L68) AND L26
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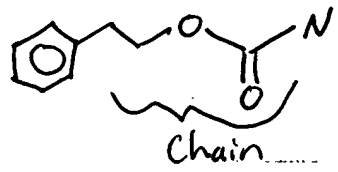
L26 →



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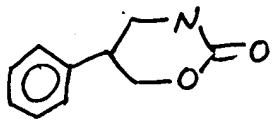

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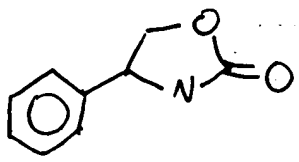
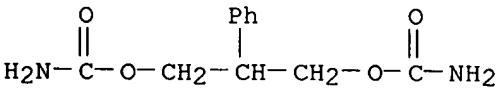
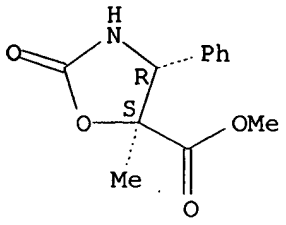


L70 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 2001:490075 HCAPLUS
DN 135:204893
TI The Chemistry, Toxicology, and Identification in Rat and Human Urine of 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one: A Reactive Metabolite in Felbamate Bioactivation
AU Dieckhaus, Christine M.; Santos, Webster L.; Sofia, R. Duane; Macdonald, Timothy L.
CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901, USA
SO Chem. Res. Toxicol. (2001), 14(8), 958-964
CODEN: CRTOEC; ISSN: 0893-228X
PB American Chemical Society
DT Journal
LA English
AB 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one has been proposed to be a reactive metabolite of the anti-epileptic drug felbamate. 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one exists in equil. with 3-oxo-2-phenylpropyl aminooate, which is known to eliminate to generate 2-phenylpropenal. Thus, this species is postulated to be a latent form of the ultimate reactive metabolite, 2-phenylpropenal. The chem. of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is proposed to parallel that of 4-hydroxycyclophosphamide, the bioactivated form of cyclophosphamide that undergoes ring-opening to aldophosphamide and subsequent elimination to afford 2-propenal (acrolein). The work presented here reports the chem. synthesis of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one and demonstrates that under buffered conditions it exists in equil. with 3-oxo-2-phenylpropyl aminooate. The rate-limiting step in the decompn. of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is the irreversible .beta.-elimination from 3-oxo-2-phenylpropyl aminooate to 2-phenylpropenal. We have found the half-life of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one to be 4.6.+-.0.4 h under in vitro conditions that mimic the physiol. setting. As a consequence of the relatively long half-life of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one, we have sought evidence for the significance of this pathway in exptl. and clin. conditions. We report here the observation of this metabolite in the urine of rats being treated with 3-hydroxy-2-phenylpropyl aminooate, the esterase-mediated metabolite of felbamate, and in the urine of patients undergoing felbamate therapy. In addn., we have shown that 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is toxic to cultured cells in a time-dependent manner, most likely as a result of its decompn. to 2-phenylpropenal. Taken together, the data support the hypothesis that 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one represents a "time-release" form of 2-phenylpropenal capable of traveling to distal sites from its locus of bioactivation and thereby mediates felbamate assocd. toxicities.
IT **25451-15-4**, Felbamate
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(chem., toxicol., and identification in rat and human urine of a reactive metabolite in felbamate bioactivation)
RN 25451-15-4 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)

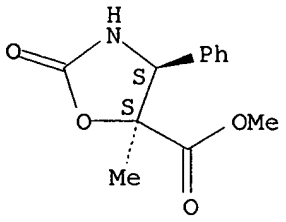


2 of 4 Inventors



RN 335200-12-9 HCAPLUS
CN 5-Oxazolidinecarboxylic acid, 5-methyl-2-oxo-4-phenyl-, methyl ester, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 65
RE
(1) Ager, D; Aldrichimica Acta 1997, V30, P3 HCAPLUS
(2) Ager, D; Chem Rev 1996, V96, P835 HCAPLUS
(3) Albone, D; J Org Chem 1998, V63, P9569 HCAPLUS
(4) Au, S; Chem Commun 1998, P2677 HCAPLUS
(5) Au, S; J Am Chem Soc 1999, V121, P9120 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 2000:573661 HCAPLUS
DN 133:172201
TI Felbamate derived compounds
IN MacDonald, Timothy L.; Miller, Thomas A.; Thompson, Charles D.
PA University of Virginia Patent Foundation, USA
SO PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000047202	A1	20000817	WO 2000-US3147	20000208

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

3 of 4
← Inventors

RN 288302-37-4 HCAPLUS
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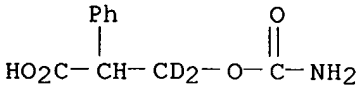
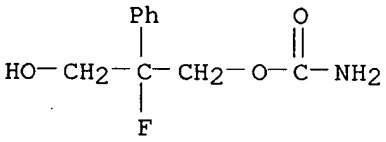
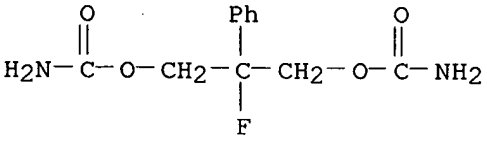


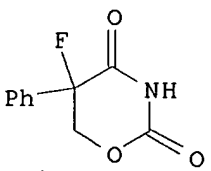
IT **288302-42-1P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)
RN 288302-42-1 HCAPLUS
CN 1,3-Propanediol, 2-fluoro-2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)

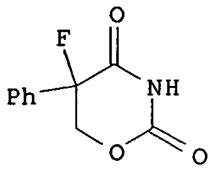


IT **726-99-8P 288302-44-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)
RN 726-99-8 HCAPLUS
CN 1,3-Propanediol, 2-fluoro-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)

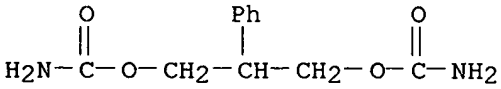


RN 288302-44-3 HCAPLUS
CN 2H-1,3-Oxazine-2,4(3H)-dione, 5-fluorodihydro-5-phenyl- (9CI) (CA INDEX NAME)

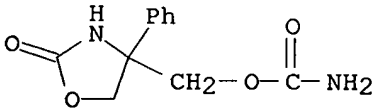




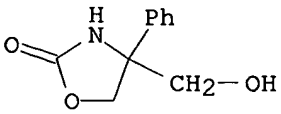
IT **25451-15-4D**, Felbamate, derivs. **288302-40-9**
288302-41-0
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)
RN 25451-15-4 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



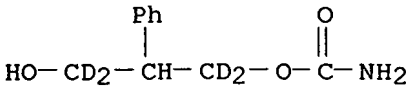
RN 288302-40-9 HCAPLUS
CN 2-Oxazolidinone, 4-[[(aminocarbonyl)oxy]methyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 288302-41-0 HCAPLUS
CN 2-Oxazolidinone, 4-(hydroxymethyl)-4-phenyl- (9CI) (CA INDEX NAME)



IT **288302-36-3P 288302-43-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)
RN 288302-36-3 HCAPLUS
CN 1,3-Propane-1,1,3,3-d4-diol, 2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)



RN 288302-43-2 HCAPLUS
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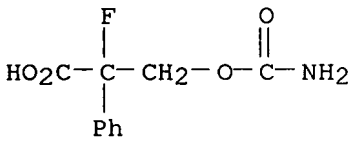
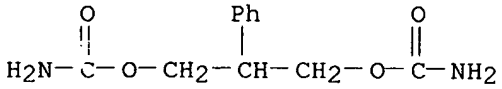


RE.CNT 2
RE
(1) Choi; 1987, 2, P705 HCAPLUS
(2) Choi; Tetrahedron 1986, V42(23), P6399 HCAPLUS

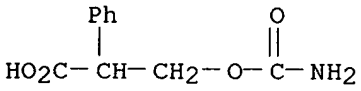
L70 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 2000:213938 HCAPLUS
DN 132:342749
TI The synthesis, in vitro reactivity, and evidence for formation in humans of 5-phenyl-1,3-oxazinane-2,4-dione, a metabolite of felbamate
AU Thompson, Charles D.; Miller, Thomas A.; Barthen, Mary T.; Dieckhaus, Christine M.; Sofia, R. Duane; Macdonald, Timothy L.
CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901, USA
SO Drug Metab. Dispos. (2000), 28(4), 434-439
CODEN: DMDSAI; ISSN: 0090-9556
PB American Society for Pharmacology and Experimental Therapeutics
DT Journal
LA English
AB Previously we have proposed and provided evidence for a metabolic scheme leading to 3-carbamoyl-2-phenylpropionaldehyde from the antiepileptic drug felbamate. This aldehyde was found to undergo reversible cyclization to form the more stable cyclic carbamate 4-hydroxy-5-phenyl-tetrahydro-1,3-oxazin-2-one or undergo elimination to form 2-phenylpropenal. The cyclic carbamate bears structural similarity to 4-hydroxycyclophosphamide and there is an intriguing parallelism between the pathway from the cyclic carbamate to 2-phenylpropenal and the known pathway from 4-hydroxycyclophosphamide to acrolein. The similarity of these transformations led us to consider 5-phenyl-1,3-oxazinane-2,4-dione, which could arise from an oxidn. of the cyclic carbamate, as a potential metabolite of felbamate. As the formation of this dione species may have both potential pharmacol. and toxicol. implications for felbamate therapy, we wished to study its reactivity. We have developed a synthesis of 5-phenyl-1,3-oxazinane-2,4-dione and evaluated its reactivity in vitro. This dione was found to undergo base-catalyzed decompn. to three products, one of which is the major human metabolite of felbamate, 3-carbamoyl-2-phenylpropionic acid. Furthermore, we have found evidence for the presence of the dione in human urine after felbamate treatment through the identification of its major in vitro decompn. product, 2-phenylacrylamide 11.

All 4 Inventors

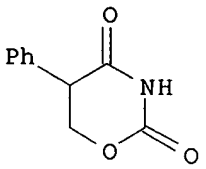
IT **25451-15-4**, Felbamate
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(synthesis, in vitro reactivity, and evidence for formation in humans of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)
RN 25451-15-4 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



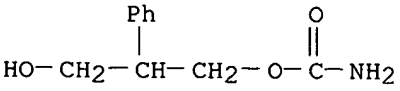
IT **139262-66-1P**
RL: FMU (Formation, unclassified); RCT (Reactant); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(synthesis, in vitro reactivity, and evidence for formation in humans of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)
RN 139262-66-1 HCAPLUS
CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)

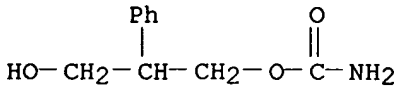


IT **269062-79-5P**
RL: MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(synthesis, in vitro reactivity, and evidence for formation in humans of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)
RN 269062-79-5 HCAPLUS
CN 2H-1,3-Oxazine-2,4(3H)-dione, dihydro-5-phenyl- (9CI) (CA INDEX NAME)



IT **25451-53-0**
RL: RCT (Reactant)
(synthesis, in vitro reactivity, and evidence for formation in humans of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)
RN 25451-53-0 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



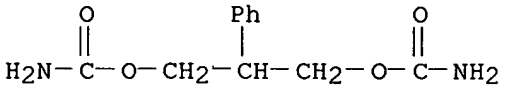


RE.CNT 12
RE
(1) Adusumalli, V; Drug Metab Dispos 1993, V21, P710 HCAPLUS
(2) Kapetanovic, I; Drug Metab Dispos 1998, V26, P1089 HCAPLUS
(5) Takamizawa, A; Chem Pharm Bull (Tokyo 1972, V20, P1612 HCAPLUS
(6) Testa, E; J Org Chem 1959, V24, P1928 HCAPLUS
(7) Thompson, C; Chem Res Toxicol 1996, V9, P1225 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1998:725893 HCAPLUS
DN 130:104748
TI Potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro
AU Kapetanovic, Izet M.; Torchin, Cynthia D.; Thompson, Charles D.; Miller, Thomas A.; McNeilly, Patrick J.; MacDonald, Timothy L.; Kupferberg, Harvey J.; Perhach, James L.; Sofia, R. Duane; Strong, John M.
CS Epilepsy Branch, National Institute of Neurological Disorders and Stroke, USA
SO Drug Metab. Dispos. (1998), 26(11), 1089-1095
CODEN: DMDSAI; ISSN: 0090-9556
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Felbamate (FBM) is a novel antiepileptic drug that was approved in 1993 for treatment of several forms of epilepsy. After its introduction, toxic reactions (aplastic anemia and hepatotoxicity) assocd. with its use were reported. It is unknown whether FBM or one of its metabolites is responsible for these idiosyncratic adverse reactions. Although the metab. of FBM has not been fully characterized, three primary metabolites of FBM have been identified, i.e. 2-hydroxy, p-hydroxy, and monocarbamate metabolites. In addn., the monocarbamate metabolite leads to a carboxylic acid, which is the major metabolite of FBM in humans. Formation of the hydroxylated products of FBM involves cytochrome P 450 enzymes, but the enzymes involved in the formation and further metab. of the monocarbamate have not yet been elucidated. Recently, mercapturate metabolites of FBM have been identified in human urine, and a metabolic scheme involving reactive aldehyde metabolite formation from the monocarbamate metabolite has been proposed. The present study confirmed the formation of the proposed metabolites using human liver tissue in vitro. The aldehyde intermediates were trapped as oxime derivs., and the cyclic equil. product (proposed as a storage and transport form for the aldehydes) was monitored directly by HPLC or GC/MS. Formation of putative toxic aldehyde intermediates and the major carboxylic acid metabolite of FBM was differentially effected with the cofactors NADP+ and NAD+. It is possible that the cofactors may influence the relative metab. via activation and inactivation pathways.
IT **25451-15-4**, Felbamate **25451-53-0**, 2-Phenyl-1,3-propanediol monocarbamate
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)

3 of 4

RN 25451-15-4 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



RN 25451-53-0 HCAPLUS
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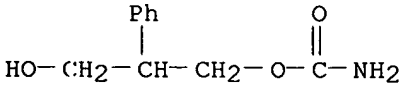
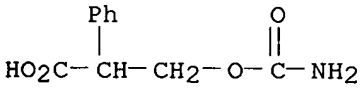
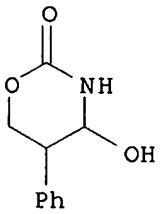


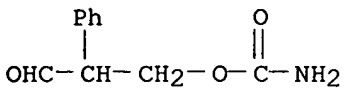
IT **139262-66-1 183961-08-2**
RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)
RN 139262-66-1 HCAPLUS
CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



RN 183961-08-2 HCAPLUS
CN 2H-1,3-Oxazin-2-one, tetrahydro-4-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)



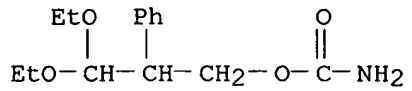
IT **183961-07-1**
RL: MFM (Metabolic formation); RCT (Reactant); BIOL (Biological study); FORM (Formation, nonpreparative)
(potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)
RN 183961-07-1 HCAPLUS
CN Benzeneacetaldehyde, .alpha.-[[(aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



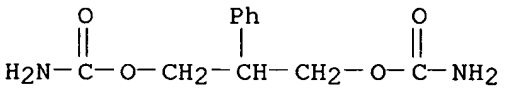
RE.CNT 17
RE
(1) Adusumalli, V; Drug Metab Dispos 1993, V21, P710 HCAPLUS
(2) Anderson, L; J Chromatogr 1995, V667, P247 HCAPLUS
(3) Glue, P; Clin Pharmacokine 1997, V33, P214 HCAPLUS
(4) Guengerich, F; Chem Res Toxicol 1991, V4, P413 HCAPLUS
(5) Ingelman-Sundberg, M; Exper Suppl 1994, V71, P197 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1996:664849 HCAPLUS
DN 126:300
TI Synthesis and in Vitro Reactivity of 3-Carbamoyl-2-phenylpropionaldehyde and 2-Phenylpropenal: Putative Reactive Metabolites of Felbamate
AU Thompson, Charles D.; Kinter, Michael T.; Macdonald, Timothy L.
CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901, USA
SO Chem. Res. Toxicol. (1996), 9(8), 1225-1229
CODEN: CRTOEC; ISSN: 0893-228X
PB American Chemical Society
DT Journal
LA English
AB We propose that 3-carbamoyl-2-phenylpropionaldehyde is an intermediate in the metab. of felbamate, an anti-epileptic drug with a unique profile of therapeutic activity, and undergoes a cascade of chem. reactions responsible for the toxic properties of the parent drug. To test this hypothesis, we have synthesized 3-carbamoyl-2-phenylpropionaldehyde and evaluated its in vitro reactivity. This mol. was found to be highly unstable at physiol. pH (t1/2 .ltoreq. 30 s) and to undergo facile elimination to 2-phenylpropenal, an .alpha.,.beta.-unsatd. aldehyde commonly termed atropaldehyde. However, the predominant reaction pathway for 3-carbamoyl-2-phenylpropionaldehyde was reversible cyclization to generate 4-hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one, a urethane that has a considerably longer half-life at physiol. pH (t1/2 .gtoreq. 5 h) and may serve as a stable reservoir of the reactive aldehyde both in vitro and in vivo. Atropaldehyde is a potent electrophile and was found to exhibit cytotoxicity to cultured fibroblasts (50% growth inhibition (GI50) = 4.1 .+-. 1.1 .mu.M) comparable to the known unsatd. aldehyde toxins, 4-hydroxy-2-nonenal and acrolein. 3-Carbamoyl-2-phenylpropionaldehyde also exhibited significant cytotoxicity (GI50 = 53 .+-. 8 .mu.M), whereas 2-phenyl-1,3-propanediol monocarbamate (GI50 > 500 .mu.M) and 3-carbamoyl-2-phenylpropionic acid (GI50 > 500 .mu.M) were nontoxic. We have addnl. demonstrated the formation of a glutathione-atropaldehyde conjugate from the in vitro incubation of 3-carbamoyl-2-phenylpropionaldehyde with glutathione. Thus, the potent cytotoxicity and potential allergenicity of atropaldehyde implicate this unsatd. aldehyde as a possible causative agent in the toxicities obsd. with felbamate treatment.
IT **183961-10-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; synthesis and in vitro reactivity of putative toxic metabolites of felbamate)

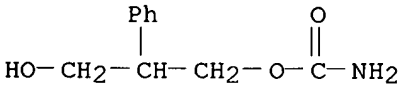
RN 183961-10-6 HCAPLUS
CN Benzeneethanol, .beta.-(diethoxymethyl)-, carbamate (9CI) (CA INDEX NAME)



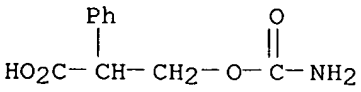
IT **25451-15-4**, Felbamate
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BIOL (Biological study); PROC (Process)
(synthesis and in vitro reactivity of putative toxic metabolites of felbamate)
RN 25451-15-4 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



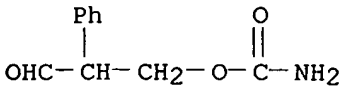
IT **25451-53-0**, 2-Phenyl-1,3-propanediol monocarbamate
139262-66-1
RL: ADV (Adverse effect, including toxicity); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(synthesis and in vitro reactivity of putative toxic metabolites of felbamate)
RN 25451-53-0 HCAPLUS
CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



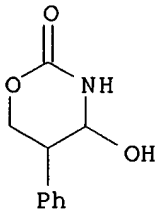
RN 139262-66-1 HCAPLUS
CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



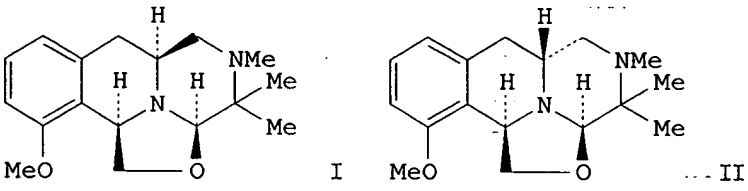
IT **183961-07-1P 183961-08-2P**
RL: MFM (Metabolic formation); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(synthesis and in vitro reactivity of putative toxic metabolites of felbamate)
RN 183961-07-1 HCAPLUS
CN Benzeneacetaldehyde, .alpha.-[[(aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



RN 183961-08-2 HCAPLUS
CN 2H-1,3-Oxazin-2-one, tetrahydro-4-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)

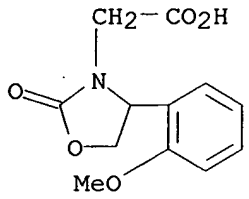


L70 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1991:428963 HCAPLUS
DN 115:28963
TI Synthesis, conformation, crystal structures and DNA cleavage abilities of tetracyclic analogs of quinocarcin
AU Williams, Robert M.; Glinka, Tomasz; Gallegos, Renee; Ehrlich, Paul P.; Flanagan, Mark E.; Coffman, Hazel; Park, Gyoosoon
CS Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
SO Tetrahedron (1991), 47(14-15), 2629-42
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI

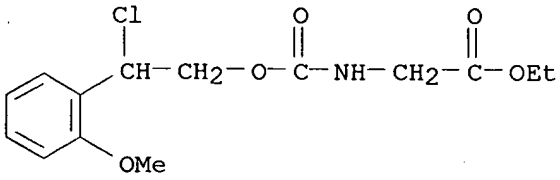


AB Racemic tetracyclic quinocarcin analogs I and II were prepd. and their DNA cleaving abilities investigated. Both substances effect the modest cleavage of plasmid DNA. Alteration of the conformation of the reactive oxazolidine fused to the piperazine ring by selecting the stereochem. at C-11a drastically attenuated the relative ability of these substances to cleave DNA.
IT **108343-93-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and intramol. acylation of, isoquinoline from)
RN 108343-93-7 HCAPLUS

CN 3-Oxazolidineacetic acid, 4-(2-methoxyphenyl)-2-oxo- (9CI) (CA INDEX NAME)



IT **134307-60-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and intramol. cyclocondensation of, oxazole from)
RN 134307-60-1 HCAPLUS
CN Glycine, N-[[2-chloro-2-(2-methoxyphenyl)ethoxy]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



L70 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1990:669 HCAPLUS
DN 112:669
TI Amino acid derivatives, processes for their preparation, and pharmaceutical compositions comprising them for treatment of hypertension and heart failure
IN Hemmi, Keiji; Neya, Masahiro; Marusawa, Hiroshi; Imai, Keisuke; Kayakiri, Natsuko; Hashimoto, Masashi
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO Eur. Pat. Appl., 60 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 300189	A2	19890125	EP 1988-109430	19880614
	EP 300189	A3	19900822		
	EP 300189	B1	19941102		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8804087	A	19890222	ZA 1988-4087	19880608
	US 4921855	A	19900501	US 1988-204549	19880609
	ES 2067456	T3	19950401	ES 1988-109430	19880614
	FI 8802875	A	19881223	FI 1988-2875	19880616
	FI 96202	B	19960215		
	FI 96202	C	19960527		
	IL 86782	A1	19930404	IL 1988-86782	19880616

	AU 8818190	A1	19881222	AU 1988-18190	19880621
	AU 617674	B2	19911205		
	DK 8803400	A	19881223	DK 1988-3400	19880621
	NO 8802732	A	19881223	NO 1988-2732	19880621
	NO 175371	B	19940627		
	NO 175371	C	19941005		
	CN 1030411	A	19890118	CN 1988-103878	19880621
	CN 1026892	B	19941207		
	JP 01019071	A2	19890123	JP 1988-153041	19880621
	JP 06025147	B4	19940406		
	HU 47917	A2	19890428	HU 1988-3164	19880621
	HU 202212	B	19910228		
	SU 1801107	A3	19930307	SU 1988-4356019	19880621
	US 5142048	A	19920825	US 1990-462117	19900108
	RU 2070195	C1	19961210	RU 1991-5010142	19911122
	US 5223489	A	19930629	US 1992-828193	19920130
PRAI	GB 1987-14597		19870622		
	GB 1987-25511		19871030		
	GB 1988-5389		19880307		
	US 1988-204549		19880609		
	US 1990-462117		19900108		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A process for prepg. I [R1 = lower alkyl optionally substituted with acyl, hydroxy, lower alkoxy, aryl, lower alkylthio, NR5R6; R5 = H, acyl; R6 = H, lower alkyl, aryl, (lower alkyl- or acyl-substituted) amino; R2, R3 = H, lower alkyl; R4 = lower alkyl; R1NR2 = heterocycle optionally substituted with lower alkyl, hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, acyl(lower)alkyl, oxo, acyl] or its pharmaceutically acceptable salt comprises (a) reacting II (R3, R4 as above; R8 = H, N-protective group) or its reactive deriv. at the amino group or a salt thereof with III (R1, R2 as above) or its reactive deriv. at the COO group or a salt thereof, and, if necessary, eliminating the N-protective group or (b) subjecting IV (R2, R3, R4, R6 as above; R7 = N-protective group; A = lower alkylene) or its salt to elimination reaction of R7 to give V (R2, R3, R4, R6, A as above) or its salt. I are useful as antihypertensives or for the treatment of heart failure. A soln. of 2(S)-[N-(2-morpholinocarbonylethyl)-N-methylaminocarbonyloxy]-3-phenylpropionic acid (prepn. described) 449 and 2(S)-(N.alpha.-methyl-Nim-tosyl-L-histidyl)amino-1-cyclohexyl-3(S)-hydroxy-6-methylheptane (prepn. described) 300 mg in CH2Cl2 (30 mL) was mixed with N-ethyl-N'-(3-dimethylaminopropyl)carbodiimide-HCl 140 mg at 5.degree. overnight. The residue was dissolved in EtOAC, washed with HCl/NaHCO3, dried, redissolved in DMF, and reacted with pyridine-HCl 650 mg for 2 h at room temp. Workup and purifn. by TLC yielded 2(S)-[N.alpha.-[2(S)-[N-(2-morpholinocarbonylethyl)-N-methylaminocarbonyloxy]-3-phenylpropionyl]-N.alpha.-methyl-L-histidyl]amino-1-cyclohexyl-3(S)-hydroxy-6-methylheptane (VI) 221 mg (m.p. 80-87.degree.) as an amorphous powder. VI, dissolved in HCl and orally administered to Na-depleted male or female cynomolgus monkeys (32 mg/kg), reduced mean arterial blood pressure and plasma renin activity by 18 and 92%, resp.

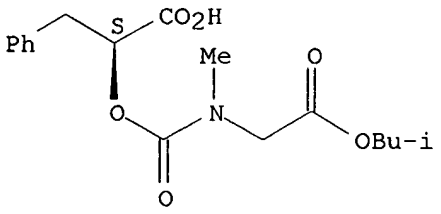
IT **124074-67-5P 124074-69-7P 124074-70-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, in antihypertensive amino acid deriv. prepn.)

RN 124074-67-5 HCAPLUS

CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, 2-methylpropyl ester, (S)- (9CI) (CA INDEX NAME)

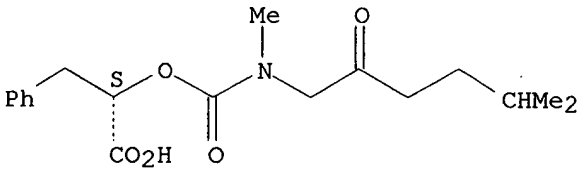
Absolute stereochemistry.



RN 124074-69-7 HCAPLUS

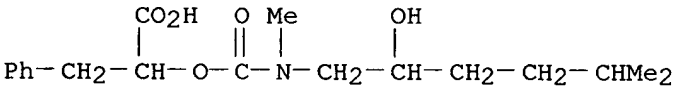
CN Benzenepropanoic acid, .alpha.-[[[methyl(5-methyl-2-oxohexyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124074-70-0 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[(2-hydroxy-5-methylhexyl)methylamino]carbonyl]oxy]- (9CI) (CA INDEX NAME)

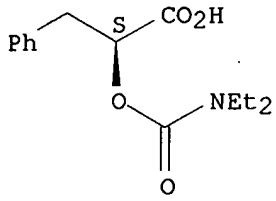


IT **124074-43-7P 124074-44-8P 124074-45-9P**
124074-46-0P 124074-48-2P 124074-51-7P
124074-57-3P 124074-59-5P 124074-60-8P
124074-71-1P 124074-72-2P 124074-79-9P
124074-82-4P 124074-84-6P 124074-86-8P
124074-87-9P 124074-89-1P 124074-90-4P
124074-93-7P 124074-96-0P 124074-97-1P
124074-98-2P 124075-01-0P 124075-02-1P
124075-05-4P 124075-08-7P 124075-09-8P
124075-28-1P 124075-33-8P 124075-36-1P
124075-37-2P 124075-38-3P 124122-50-5P
124122-51-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, in prepn. of antihypertensives)

RN 124074-43-7 HCAPLUS

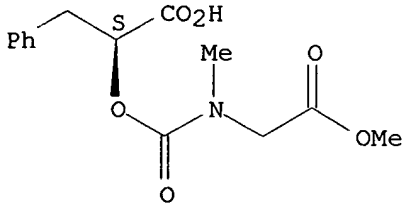
CN Benzenepropanoic acid, .alpha.-[[(diethylamino)carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



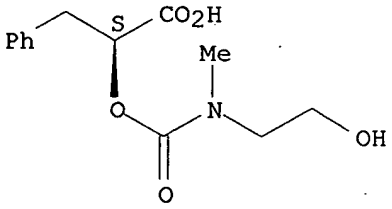
RN 124074-44-8 HCAPLUS
CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



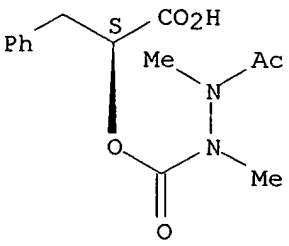
RN 124074-45-9 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[(2-hydroxyethyl)methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

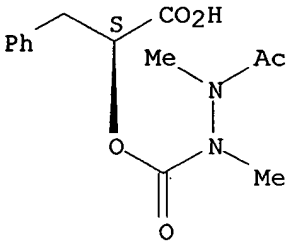
Absolute stereochemistry.



RN 124074-46-0 HCAPLUS
CN Hydrazinecarboxylic acid, 2-acetyl-1,2-dimethyl-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

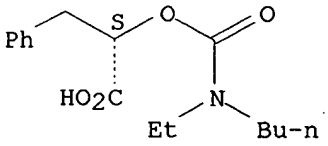
Absolute stereochemistry.





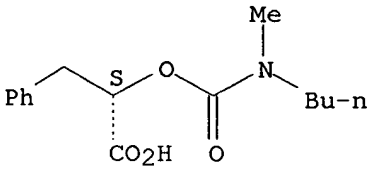
RN 124074-48-2 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[(butylethylamino)carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



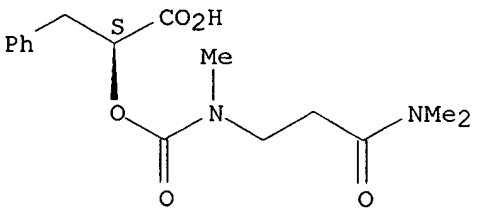
RN 124074-51-7 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[(butylmethylamino)carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



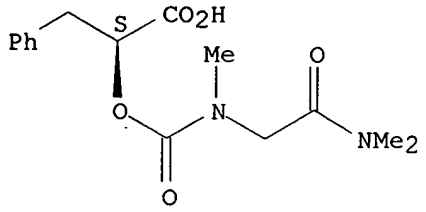
RN 124074-57-3 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[[3-(dimethylamino)-3-oxopropyl]methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



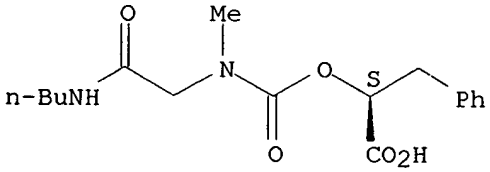
RN 124074-59-5 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[[2-(dimethylamino)-2-oxoethyl]methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



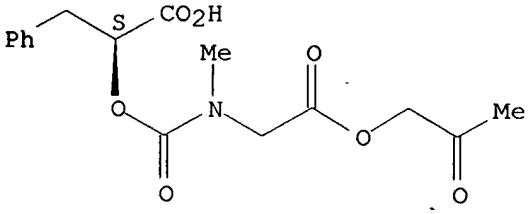
RN 124074-60-8 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[[2-(butylamino)-2-oxoethyl]methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



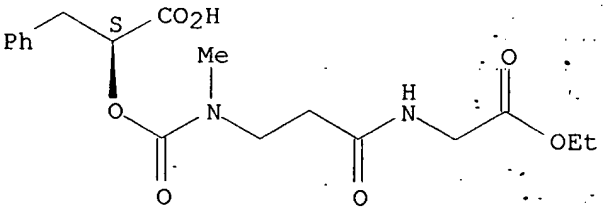
RN 124074-71-1 HCAPLUS
CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, 2-oxopropyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124074-72-2 HCAPLUS
CN Glycine, N-[N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-.beta.-alanyl]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

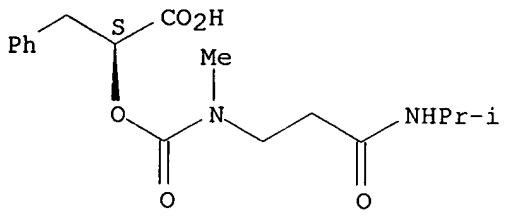
Absolute stereochemistry.



RN 124074-79-9 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(1-methylethyl)amino]-3-

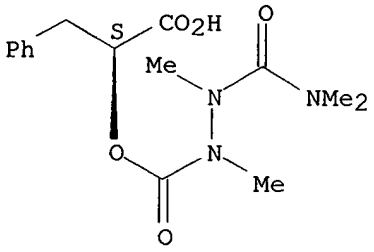
oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



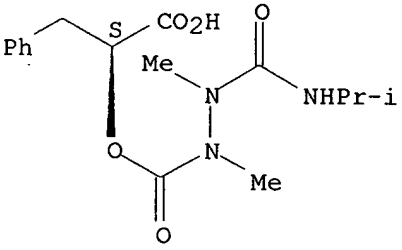
RN 124074-82-4 HCAPLUS
CN Hydrazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-1,2-dimethyl-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



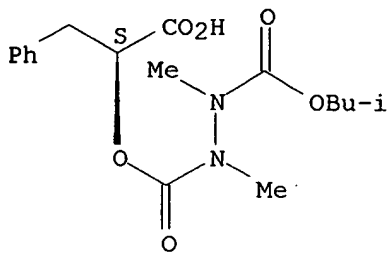
RN 124074-84-6 HCAPLUS
CN Hydrazinecarboxylic acid, 1,2-dimethyl-2-[[(1-methylethyl)amino]carbonyl]-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



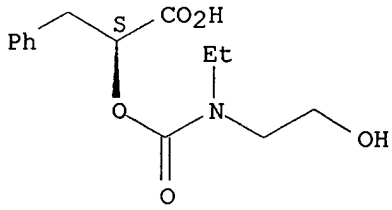
RN 124074-86-8 HCAPLUS
CN 1,2-Hydrazinedicarboxylic acid, 1,2-dimethyl-, 1-carboxy-2-phenylethyl 2-methylpropyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



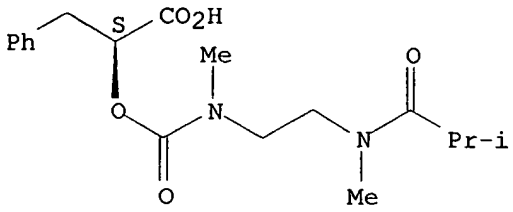
RN 124074-87-9 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[ethyl(2-hydroxyethyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



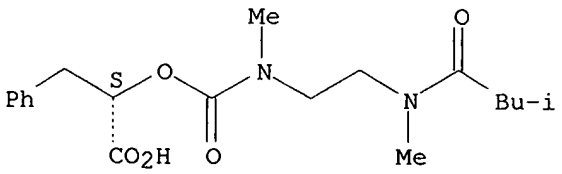
RN 124074-89-1 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[methyl(2-methyl-1-oxopropyl)amino]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124074-90-4 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[methyl(3-methyl-1-oxobutyl)amino]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

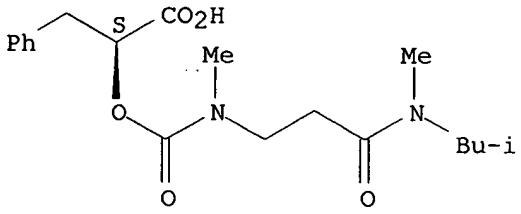
Absolute stereochemistry.



RN 124074-93-7 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[methyl(2-methylpropyl)amino]-3-

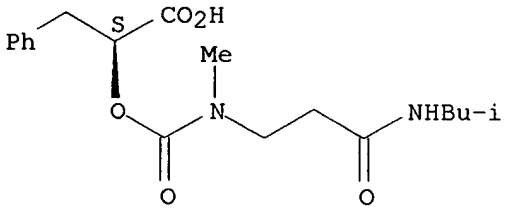
oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



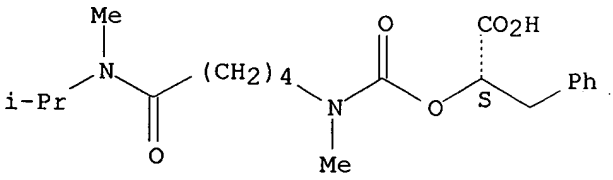
RN 124074-96-0 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)amino]-3-oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



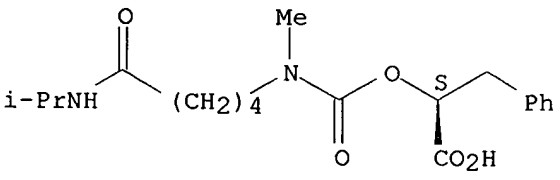
RN 124074-97-1 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[5-[methyl(1-methylethyl)amino]-5-oxopentyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124074-98-2 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[5-[(1-methylethyl)amino]-5-oxopentyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

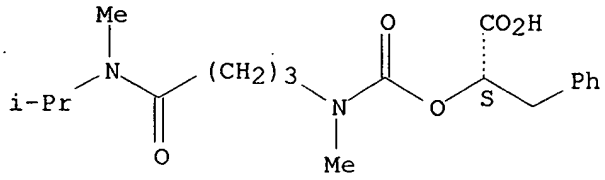
Absolute stereochemistry.



RN 124075-01-0 HCAPLUS

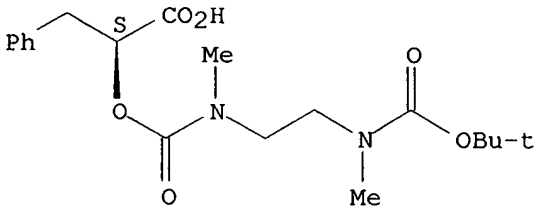
CN Benzenepropanoic acid, .alpha.-[[[methyl[4-[methyl(1-methylethyl)amino]-4-oxobutyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



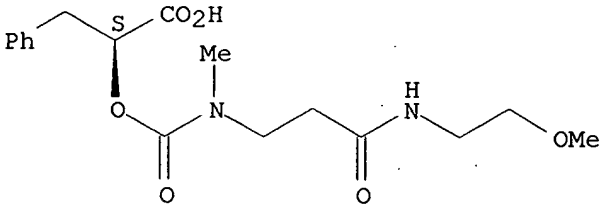
RN 124075-02-1 HCAPLUS
CN 3,10-Dioxa-5,8-diazadodecanoic acid, 5,8,11,11-tetramethyl-4,9-dioxo-2-(phenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



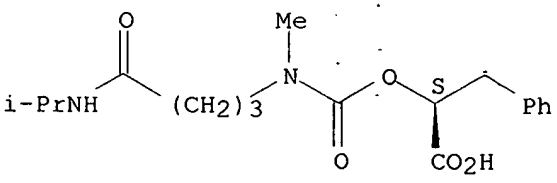
RN 124075-05-4 HCAPLUS
CN 2,11-Dioxa-5,9-diazatridecan-13-oic acid, 9-methyl-6,10-dioxo-12-(phenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



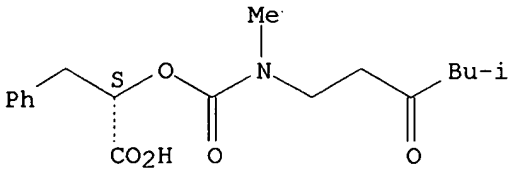
RN 124075-08-7 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[4-[(1-methylethyl)amino]-4-oxobutyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



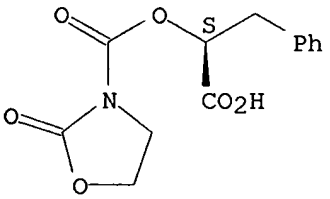
RN 124075-09-8 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl(5-methyl-3-oxohexyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



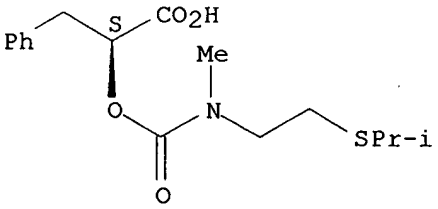
RN 124075-28-1 HCAPLUS
CN 3-Oxazolidinecarboxylic acid, 2-oxo-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



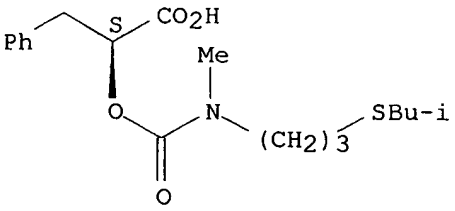
RN 124075-33-8 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[(1-methylethyl)thio]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

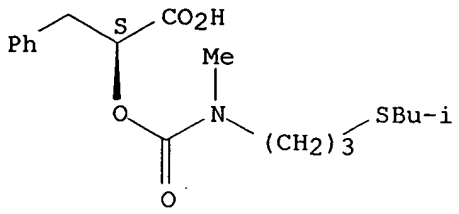
Absolute stereochemistry.



RN 124075-36-1 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)thio]propyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

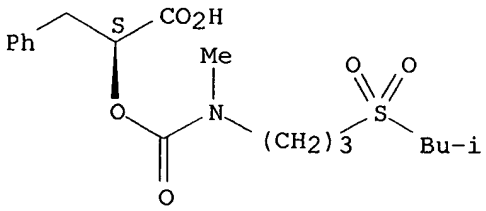
Absolute stereochemistry.





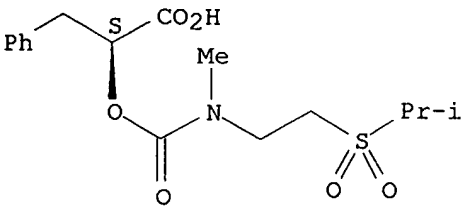
RN 124075-37-2 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)sulfonyl]propyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



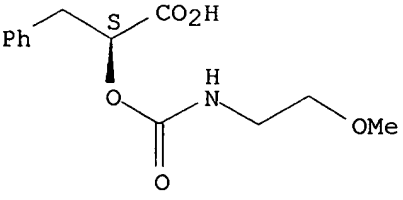
RN 124075-38-3 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[(1-methylethyl)sulfonyl]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124122-50-5 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[[(2-methoxyethyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

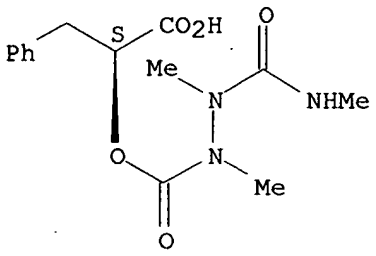
Absolute stereochemistry.



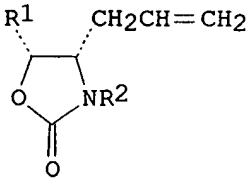
RN 124122-51-6 HCAPLUS

CN Hydrazinecarboxylic acid, 1,2-dimethyl-2-[(methylamino)carbonyl]-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

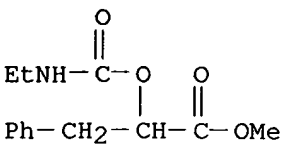


L7C ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1988:630222 HCAPLUS
DN 109:230222
TI Diastereoconversion of threo 2-amino alcohols to erythro isomers through a new cyclocarbamation
AU Kano, Shinzo; Yuasa, Yoko; Yokomatsu, Tsutomu; Shibuya, Shiroshi
CS Tokyo Coll. Pharm., Tokyo, 192-03, Japan
SO Heterocycles (1988), 27(5), 1241-8
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
OS CASREACT 109:230222
GI



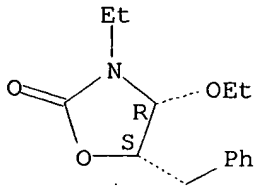
I

AB Amino alcs. threo-R1CH(OH)CH(NHR2)CH2CH:CH2 (R1 = Me, Me2CHCh2, PhCH2; R2 = Pr, PhCH2, Me, Et) were protected by (Me3CO)2CO, and the products were treated with SOCl2 to give oxazolidinones I. I are synthetic equiv. of erythro-R1CH(OH)CH(NHR2)CH2CH:CH2.
IT **117508-46-0P 117508-53-9P 117508-54-0P 117508-55-1P 117543-44-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and allylation of, by allylsilane deriv.)
RN 117508-46-0 HCAPLUS
CN Benzenepropanoic acid, .alpha.-[[(ethylamino)carbonyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)



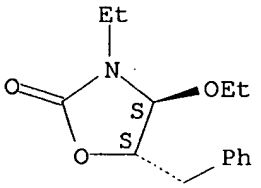
RN 117508-53-9 HCAPLUS
CN 2-Oxazolidinone, 4-ethoxy-3-ethyl-5-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



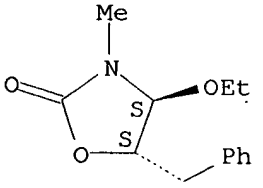
RN 117508-54-0 HCAPLUS
CN 2-Oxazolidinone, 4-ethoxy-3-ethyl-5-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



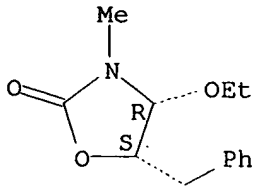
RN 117508-55-1 HCAPLUS
CN 2-Oxazolidinone, 4-ethoxy-3-methyl-5-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

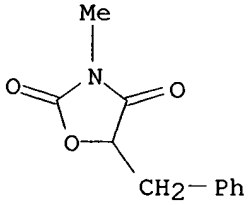


RN 117543-44-9 HCAPLUS
CN 2-Oxazolidinone, 4-ethoxy-3-methyl-5-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

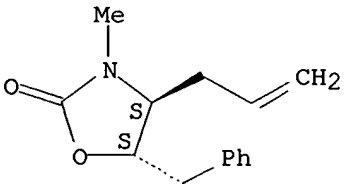


IT **5841-65-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to ethoxyoxazolidinone analog)
RN 5841-65-6 HCAPLUS
CN 2,4-Oxazolidinedione, 3-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



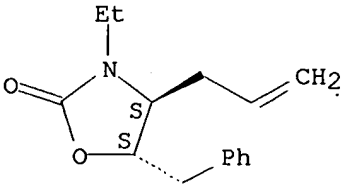
IT **117508-59-5P 117508-60-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ring cleavage of, amino alc. from)
RN 117508-59-5 HCAPLUS
CN 2-Oxazolidinone, 3-methyl-5-(phenylmethyl)-4-(2-propenyl)-, trans- (9CI)
(CA INDEX NAME)

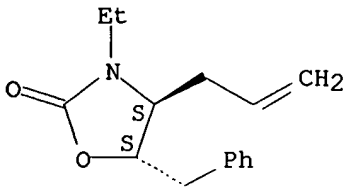
Relative stereochemistry.



RN 117508-60-8 HCAPLUS
CN 2-Oxazolidinone, 3-ethyl-5-(phenylmethyl)-4-(2-propenyl)-, trans- (9CI)
(CA INDEX NAME)

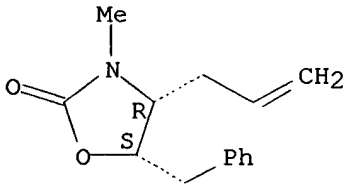
Relative stereochemistry.





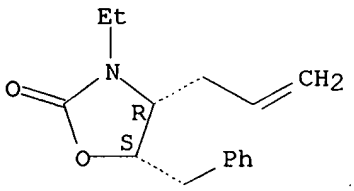
IT **117508-76-6P 117508-77-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 117508-76-6 HCAPLUS
CN 2-Oxazolidinone, 3-methyl-5-(phenylmethyl)-4-(2-propenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

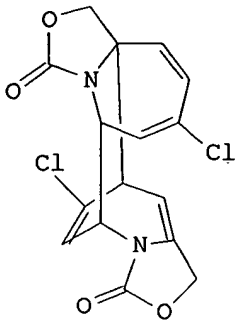


RN 117508-77-7 HCAPLUS
CN 2-Oxazolidinone, 3-ethyl-5-(phenylmethyl)-4-(2-propenyl)-, cis- (9CI) (CA INDEX NAME)

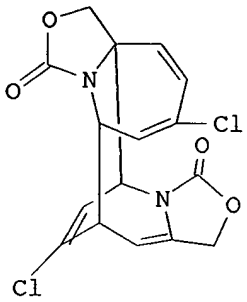
Relative stereochemistry.



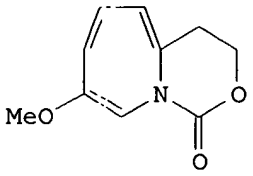
L70 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1983:178457 HCAPLUS
DN 98:178457
TI The intramolecular chemistry of benzyl and phenethyl azidoformates
AU Meth-Cohn, Otto; Patel, Dalpat; Rhouati, Salah
CS Chem. Dep., Univ. Salford, Salford, M5 4WT, UK
SO Tetrahedron Lett. (1982), 23(48), 5085-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
GI



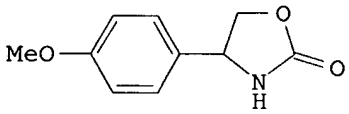
I



II



III

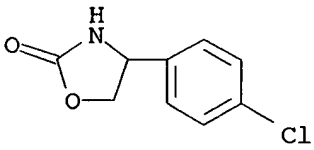


IV

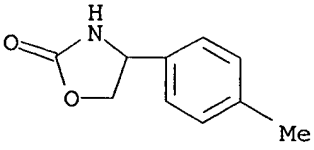
AB Benzyl azidoformates on spray pyrolysis gave, depending on the substituents present, oxazoloazepines, their syn or anti [6 + 4] dimers, their [6 + 6] dimers, benzoxazinones, or aryl isocyanates. 4-ClC6H4CH2O2CN3 on pyrolysis at 300.degree. gave a 3:2 mixt. of the syn and anti dimers I and II. Phenylethyl azidoformates on spray pyrolysis gave oxazinoazepines together with, in some cases, 4-aryloxazolidinones. Pyrolysis of 4-MeOC6H4(CH2)2O2CN3 at 300.degree. gave 61% III and 10% IV.

IT **69776-88-1P 69776-92-7P 69776-93-8P**
85288-36-4P 85288-37-5P 85288-38-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

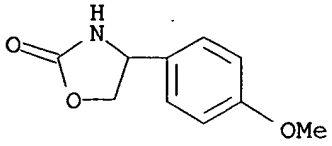
RN 69776-88-1 HCAPLUS
CN 2-Oxazolidinone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



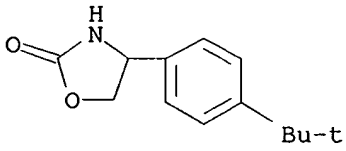
RN 69776-92-7 HCAPLUS
CN 2-Oxazolidinone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)



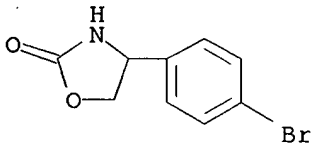
RN 69776-93-8 HCAPLUS
CN 2-Oxazolidinone, 4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



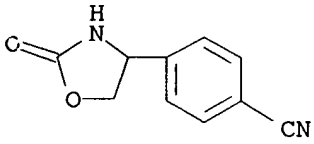
RN 85288-36-4 HCAPLUS
CN 2-Oxazolidinone, 4-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



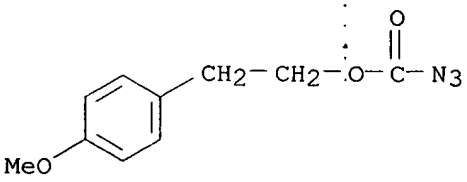
RN 85288-37-5 HCAPLUS
CN 2-Oxazolidinone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)

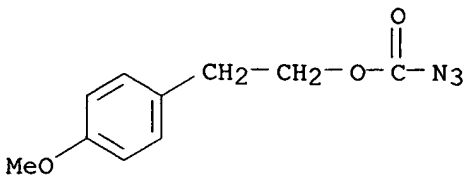


RN 85288-38-6 HCAPLUS
CN Benzonitrile, 4-(2-oxo-4-oxazolidinyl)- (9CI) (CA INDEX NAME)

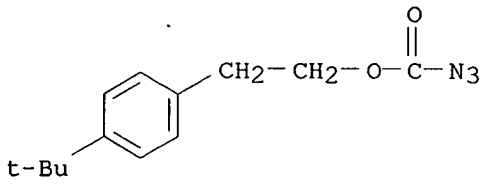


IT **85288-24-0 85288-25-1 85288-26-2**
85288-27-3 85288-28-4 85288-29-5
85288-30-8
RL: RCT (Reactant)
(pyrolysis of)
RN 85288-24-0 HCAPLUS
CN Carbonazidic acid, 2-(4-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

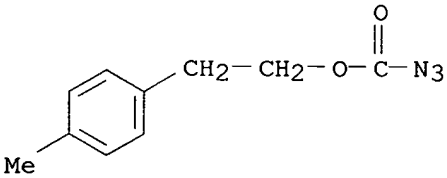




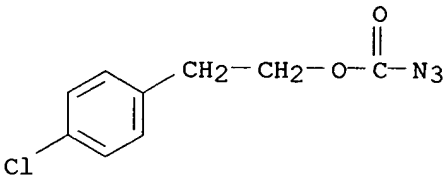
RN 85288-25-1 HCAPLUS
CN Carbonazidic acid, 2-[4-(1,1-dimethylethyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)



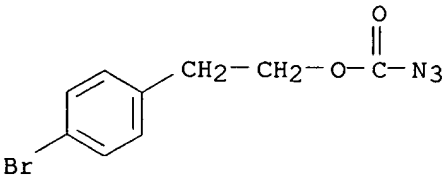
RN 85288-26-2 HCAPLUS
CN Carbonazidic acid, 2-(4-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)



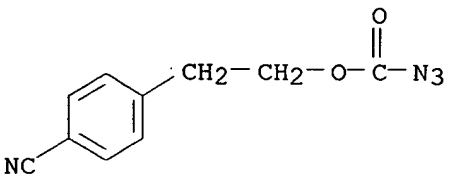
RN 85288-27-3 HCAPLUS
CN Carbonazidic acid, 2-(4-chlorophenyl)ethyl ester (9CI) (CA INDEX NAME)



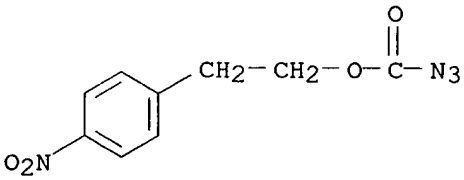
RN 85288-28-4 HCAPLUS
CN Carbonazidic acid, 2-(4-bromophenyl)ethyl ester (9CI) (CA INDEX NAME)



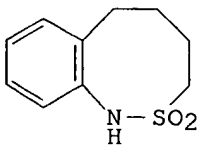
RN 85288-29-5 HCAPLUS
CN Carbonazidic acid, 2-(4-cyanophenyl)ethyl ester (9CI) (CA INDEX NAME)



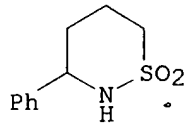
RN 85288-30-8 HCAPLUS
CN Carbonazidic acid, 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



L70 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1982:68493 HCAPLUS
DN 96:68493
TI Pyrolysis of phenylalklysulfonyl azides and 2-phenethyl azidoformate. Selectivity of sulfonylnitrenes and contrast between sulfonyl- and carbonylnitrenes
AU Abramovitch, Rudolph A.; Hendi, Shivakumar B.; Kress, Albert O.
CS Dep. Chem. Geol., Clemson Univ., Clemson, SC, 29631, USA
SO J. Chem. Soc., Chem. Commun. (1981), (20), 1087-8
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
GI



IV

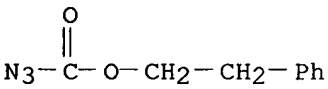


V

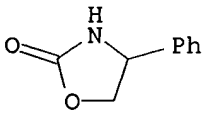
AB Flash vacuum pyrolysis (FVP) and soln. thermolysis of Ph(CH2)nSO2N3 (I; n = 3-5), and FVP of PhCH2CH2O2CN3 (II) were studied. Decompn. of I (n = 3) in Freon 113 at 135.degree. for 36 h gave 44% 2,7,8,9-tetrahydrobenzo[1,2-c]thiazepine 1,1-dioxide (III), and FVP at 990.degree. gave 72.4% 1,2,3,4-tetrahydroquinoline. Thermolysis of I (n = 4) in Freon 113 at 154.degree. for 36 h gave 30.3% of the sultam IV, whereas FVP at 710.degree. gave 17% sultam V and 7.5% E-PhCH2CH2CH:CHSO2NH2. Thermolysis

of I (n = 5) in Freon 113 at 154.degree. for 36 h gave 26% 3-benzyl-2,3,4,5,6-pentahydro-1,2-thiazine 1,1-dioxide (VI); FVP at 710.degree. gave 20.3% VI. FVP of II at 650.degree. gave 40% 4-phenyloxazolidinone and 26% tetrahydro-1,3-oxazino[3,4-a]azepin-2-one, but no dihydrocyclopenta[b]pyridine, even at 900.degree..

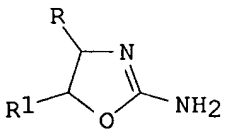
IT **80639-71-0**
RL: RCT (Reactant)
(flash vacuum pyrolysis of)
RN 80639-71-0 HCAPLUS
CN Carbonazidic acid, 2-phenylethyl ester (9CI) (CA INDEX NAME)



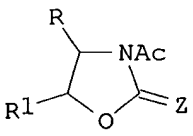
IT **7480-32-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by pyrolysis of phenethyl azidoformate)
RN 7480-32-2 HCAPLUS
CN 2-Oxazolidinone, 4-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L70 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1977:439345 HCAPLUS
DN 87:39345
TI Syntheses of oxazolecarboxylic acid derivatives. XIII. Hydrogenolysis of aminooxazoles. (6). Syntheses and hydrogenolysis of 2-amino-2-oxazolines
AU Tanaka, Chiaki; Ogata, Ikutoshi; Nishida, Motonobu
CS Osaka Coll. Pharm., Osaka, Japan
SO Yakugaku Zasshi (1977), 97(2), 157-64
CODEN: YKKZAJ
DT Journal
LA Japanese
GI



I



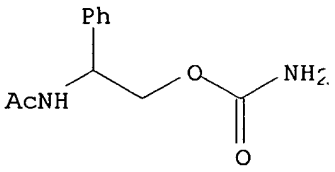
II, Z=NAc
III, Z=O

AB 2-Amino-2-oxazolines I [R = Ph, R1 = H; R = Ph, R1 = Me (cis and trans); R = Me, R1 = Ph (cis and trans)] were prepd. by the reaction of HOCHR1CHRNH2 with BrCN. Acetylation of I gave the diacetyl derivs. II rather than the monoacetyl derivs. The configuration of I was easily presumed from the

vicinal coupling const. of II. II were hydrolyzed to 3-acetyl-2-oxazolidones III and AcNHCO2CHR1CHRNHAc with 5% HCl at room temp. Catalytic redn. of I (R = Ph) gave the corresponding I (R = cyclohexyl).

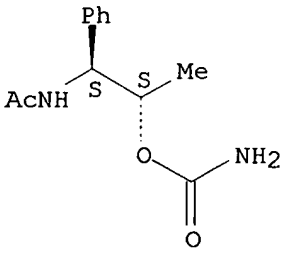
IT **63204-94-4P 63204-95-5P 63204-96-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

RN 63204-94-4 HCAPLUS
CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylethyl]- (9CI) (CA INDEX NAME)



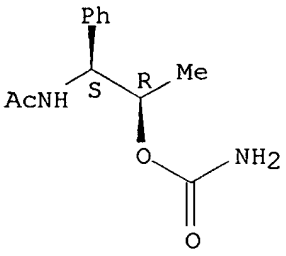
RN 63204-95-5 HCAPLUS
CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylpropyl]-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



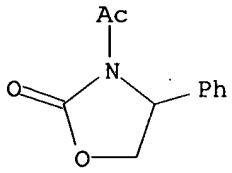
RN 63204-96-6 HCAPLUS
CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylpropyl]-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



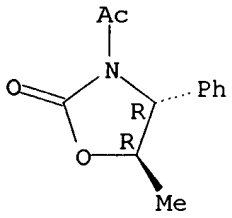
IT **63204-84-2P 63204-85-3P 63204-86-4P**
63204-89-7P 63204-90-0P 63204-91-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 63204-84-2 HCAPLUS
CN 2-Oxazolidinone, 3-acetyl-4-phenyl- (9CI) (CA INDEX NAME)



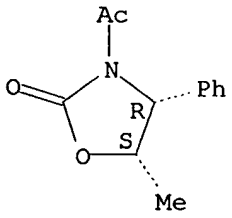
RN 63204-85-3 HCAPLUS
CN 2-Oxazolidinone, 3-acetyl-5-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

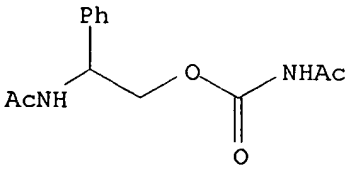


RN 63204-86-4 HCAPLUS
CN 2-Oxazolidinone, 3-acetyl-5-methyl-4-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



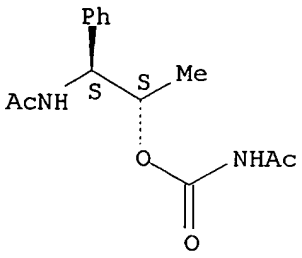
RN 63204-89-7 HCAPLUS
CN Carbamic acid, acetyl-, 2-(acetylamino)-2-phenylethyl ester (9CI) (CA INDEX NAME)



RN 63204-90-0 HCAPLUS

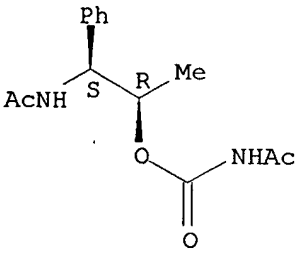
CN Carbamic acid, acetyl-, 2-(acetylamino)-1-methyl-2-phenylethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 63204-91-1 HCAPLUS
CN Carbamic acid, acetyl-, 2-(acetylamino)-1-methyl-2-phenylethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L70 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1972:540025 HCAPLUS
DN 77:140025
TI 4-Aryl-4-oxazolin-2-ones
IN Bottari, Francesco; Saettone, Marco Fabrizio; Tellini, Natale; Serafini, Maria Francesca
PA Laboratorio Guidotti e C. S.p.A.
SO Ger. Offen., 15 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3

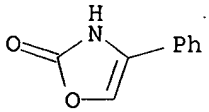
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2205676	A	19720824	DE 1972-2205676	19720207
	FR 2124468	A5	19720922	FR 1972-3740	19720204
	FR 2124468	B1	19760416		
	SE 370239	B	19741007	SE 1972-1371	19720207
	GB 1386613	A	19750312	GB 1972-5507	19720207
	ES 399572	A1	19741101	ES 1972-399572	19720208
PRAI	IT 1971-45210		19710208		

GI For diagram(s), see printed CA Issue.

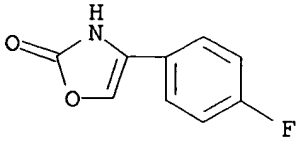
AB Ten title compds. (I, R = Ph, substituted phenyl, 1-, 2-C10H7), useful as muscle relaxants and myotonics, were prepd. by cyclization of RCOCH2O2CNH2 (II). Thus, 40 ml COCl2 (20% in PhMe) was added to 10 g PhCOCH2OH in C6H6-PhMe2 at 0.degree., the mixt. stirred 15 min at room temp., and satd. with NH3(g) at 0.degree. to give 7.55 g II (R = Ph) (III). III (5 g) was refluxed 5 hr in HOAc to give 4.2 g I (R = Ph).

IT **34375-80-9P 34375-81-0P 35961-99-0P**
35962-00-6P 35962-03-9P 35962-04-0P
35962-05-1P 35962-09-5P 35962-10-8P
35962-11-9P 35962-12-0P 36404-33-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

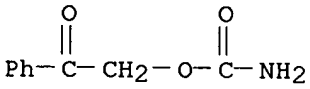
RN 34375-80-9 HCAPLUS
CN 2(3H)-Oxazolone, 4-phenyl- (9CI) (CA INDEX NAME)



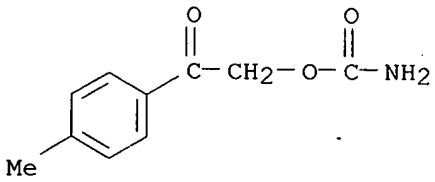
RN 34375-81-0 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



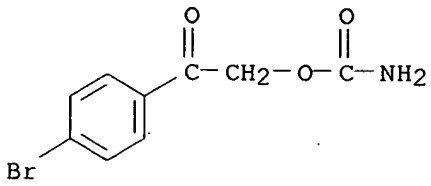
RN 35961-99-0 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



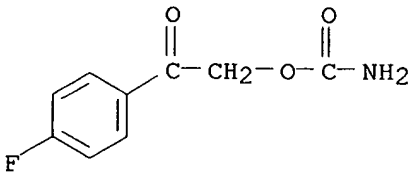
RN 35962-00-6 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-methylphenyl)- (9CI) (CA INDEX NAME)



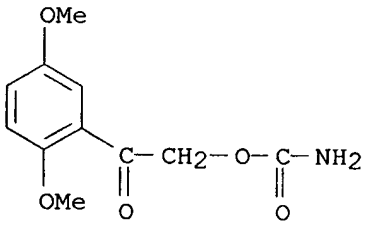
RN 35962-03-9 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)



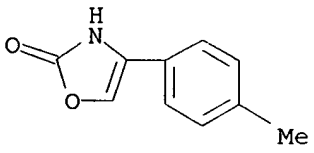
RN 35962-04-0 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



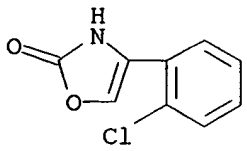
RN 35962-05-1 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



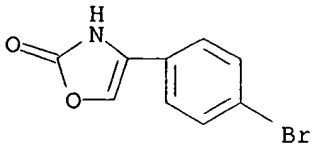
RN 35962-09-5 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)



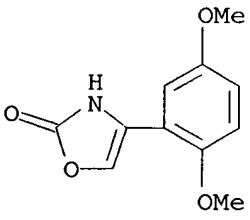
RN 35962-10-8 HCAPLUS
CN 2(3H)-Oxazolone, 4-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



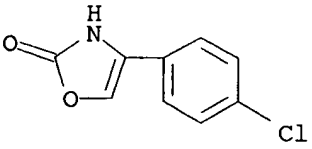
RN 35962-11-9 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)



RN 35962-12-0 HCAPLUS
CN 2(3H)-Oxazolone, 4-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 36404-33-8 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

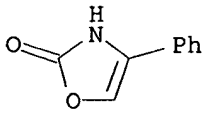


L70 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1972:108224 HCAPLUS
DN 76:108224
TI Synthesis and biological activity of some 4-aryl-substituted 4-oxazolin-2-ones
AU Bottari, Francesco; Nannipieri, Enrico; Saettone, Marco F.; Serafini, Maria F.
CS Pharm. Chem. Inst., Univ. Pisa, Pisa, Italy
SO J. Med. Chem. (1972), 15(1), 39-42
CODEN: JMCMAR
DT Journal
LA English
AB Of a series of 4-aryl-substituted 4-oxazolin-2-ones, some (group 1)

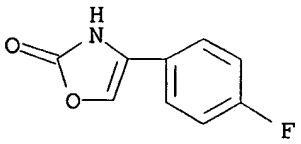
produced myotonic symptoms and antagonized barbiturate-induced sleep at dose levels of 30-100 mg/kg i.p. in mice, whereas others (group 2) showed muscle relaxant and sedative activity. Group 1 included 4-phenyl-4-oxazolin-2-one (I) [**34375-80-9**] and 4-(p-fluorophenyl)-4-oxazolin-2-one [**34375-81-0**], and group 2 included the 4-(p-biphenyl) and 4-(2-naphthyl) derivs. (III, IV). I was obtained from the relaxant drug, 2-hydroxy-2-phenylethyl carbamate (styramate) [**94-35-9**], through oxidn. and cyclization; the other compds. were prepd. similarly.

IT **34375-80-9 34375-81-0 35962-09-5 35962-10-8 35962-11-9 35962-12-0 36404-33-8**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmacology of)

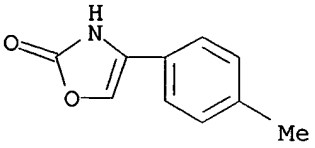
RN 34375-80-9 HCAPLUS
CN 2(3H)-Oxazolone, 4-phenyl- (9CI) (CA INDEX NAME)



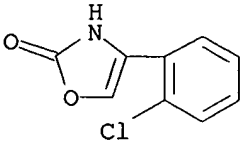
RN 34375-81-0 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



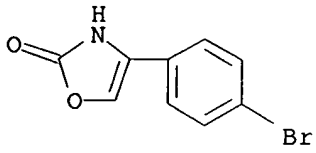
RN 35962-09-5 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)



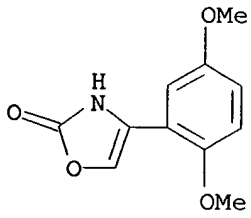
RN 35962-10-8 HCAPLUS
CN 2(3H)-Oxazolone, 4-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



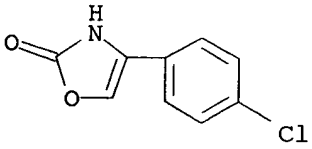
RN 35962-11-9 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)



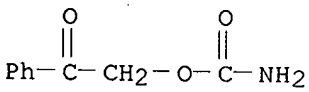
RN 35962-12-0 HCAPLUS
CN 2(3H)-Oxazolone, 4-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



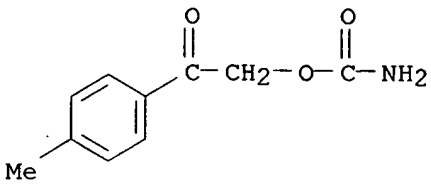
RN 36404-33-8 HCAPLUS
CN 2(3H)-Oxazolone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



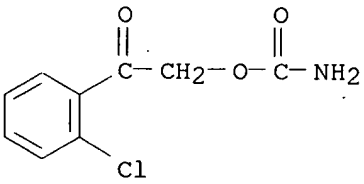
IT **35961-99-0P 35962-00-6P 35962-01-7P**
35962-02-8P 35962-03-9P 35962-04-0P
35962-05-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35961-99-0 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



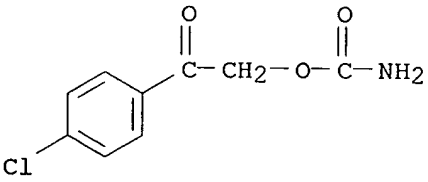
RN 35962-00-6 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-methylphenyl)- (9CI) (CA INDEX NAME)



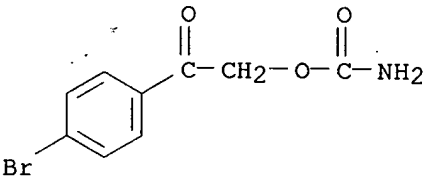
RN 35962-01-7 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



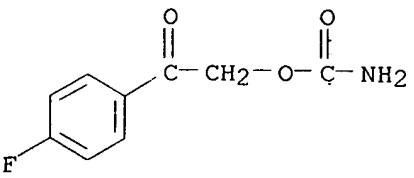
RN 35962-02-8 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

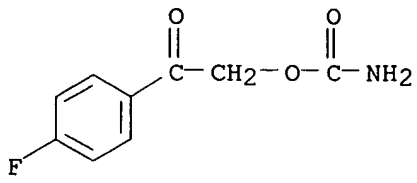


RN 35962-03-9 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)

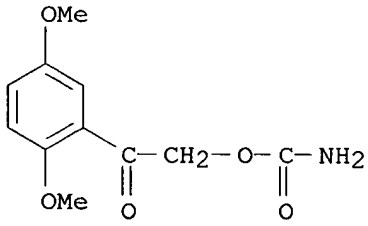


RN 35962-04-0 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

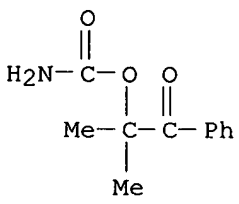




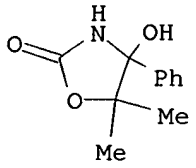
RN 35962-05-1 HCAPLUS
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



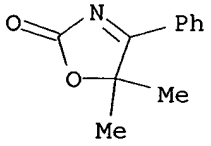
L70 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1971:488520 HCAPLUS
DN 75:88520
TI Synthesis and properties of 3-oxazol-2-ones
AU Hofmann, Hans; Wagner, Ruediger; Uhl, Juergen
CS Inst. Org. Chem., Univ. Erlangen-Nuernberg, Erlangen, Ger.
SO Chem. Ber. (1971), 104(7), 2134-42
CODEN: CHBEAM
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB RCOCR1R2OH (I), where R,R1R2 = Ph, tert-Bu, or Me or R-R2 = (CH2)5, reacted with ClSO2NCO to give RCOCR1R2O2CNH2 (II), sometimes in mixts. with the isomeric 4-hydroxyoxazolidin-2-ones. Subsequent thermal cyclization led to the corresponding 3-oxazolin-2-ones (III), which on LiAlH4 redn. yielded the oxazolidin-2-ones (IV). Alk. sapon. of IV gave I.
IT **33664-82-3P 33664-83-4P 33664-90-3P 33664-93-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 33664-82-3 HCAPLUS
CN Propiophenone, 2-hydroxy-2-methyl-, carbamate (8CI) (CA INDEX NAME)



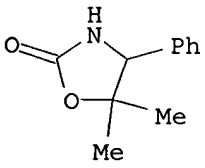
RN 33664-83-4 HCAPLUS
CN 2-Oxazolidinone, 4-hydroxy-5,5-dimethyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 33664-90-3 HCAPLUS
CN 2(5H)-Oxazolone, 5,5-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)



RN 33664-93-6 HCAPLUS
CN 2-Oxazolidinone, 5,5-dimethyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



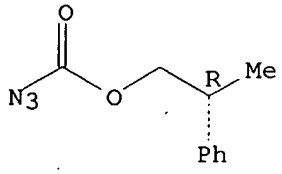
L70 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1969:36863 HCAPLUS
DN 70:36863
TI Stereochemical studies. II. Thermal and photochemical decompositions of optically active alkyl azidoformates
AU Terashima, Shiro; Yamada, Shunichi
CS Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan
SO Chem. Pharm. Bull. (Tokyo) (1968), 16(10), 1953-71
CODEN: CPBTAL
DT Journal
LA English
AB The thermal and photochem. decompns. of three types of optically active alkyl azidoformates (I) were attempted, and it was found in both cases, that optically active 2-oxazolidinones (II) were obtained with nearly complete retention of configuration. The yield of II was very low (5%) in the thermal decompn. and moderate (25-30%) in the photochem. one. Considering the relation between stereospecificity and spin multiplicity of alkoxycarbonyl nitrene, a mechanism was proposed suggesting that the singlet state alkoxycarbonyl nitrene generated from I, either by heating or by irradn., was inserted into the intramol. optically active C-H bond

through an insertion transition state. Moreover, in the course of these studies, the abs. configuration of .alpha.-methylphenylglycine (2-amino-2-phenylpropionic acid) was detd. using thermal decompn. Preliminary expts. using racemic compds. were also reported.

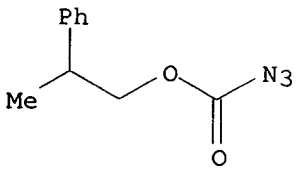
IT **13398-27-1 22436-12-0**
RL: RCT (Reactant)
(photolysis of)

RN 13398-27-1 HCAPLUS
CN Formic acid, azido-, .beta.-methylphenethyl ester, (R)-(+)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



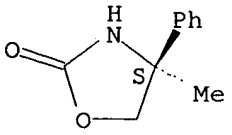
RN 22436-12-0 HCAPLUS
CN Carbonazidic acid, 2-phenylpropyl ester (9CI) (CA INDEX NAME)



IT **13398-55-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

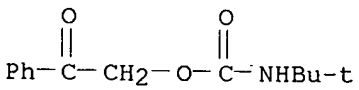
RN 13398-55-5 HCAPLUS
CN 2-Oxazolidinone, 4-methyl-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

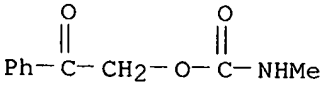


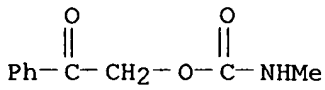
L70 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2001 ACS
AN 1967:94936 HCAPLUS
DN 66:94936
TI Carbamates. IV. Cyclization of N-substituted phenacyl carbamates to 4-hydroxyoxazolidin-2-ones and 4-oxazolin-2-ones
AU Saettone, Marco F.; Nuti, Vittorio; Da Settimo, Antonio
CS Inst. Chim. Farm., Univ. Pisa, Pisa, Italy
SO Gazz. Chim. Ital. (1966), 96(11), 1615-29

CODEN: GCITA9
DT Journal
LA Italian
GI For diagram(s), see printed CA Issue.
AB cf. CA 64, 19457f. Phenacyl alc. (6.12 g.) in 80 ml. C6H6 and 10 ml. PhNMe2 is treated at 0.degree. with 25 ml. 20% COCl2(PhMe) to give 32% phenacyl N-methylcarbamate (I), m. 106-7.degree. (C6H6-ligroine). Similarly prepd. are the following compds. of the general formula BzCH2O2CNHR (II) (R, m.p., and % yield given): Et, 105-6.degree. (C6H6-ligroine), 37; iso-Pr, 112-13.degree. (C6H6-ligroine), 55; iso-Bu, 98-100.degree. (EtOH), 50; tert-Bu, 80-1.degree. (C6H6-ligroine), 44; allyl, 88-9.degree. (C6H6-ligroine), 30; cyclopropyl, 149-51.degree. (C6H6-ligroine), 53; cyclopentyl, 129-30.degree. (EtOAc-ligroine), 66; cyclohexyl, 153-4.degree. (EtOAc-ligroine), 58; p-MeOC6H4, 158-9.degree. (C6H6-ligroine), 69. The II are refluxed with Et3N to give 4-hydroxyoxazolidin-2-ones of the general formula III and the III are refluxed with HOAc to give 4-phenyl-4-oxazolin-2-ones of the general formula IV. Thus, a soln. of 4 g. II (R = iso-Bu) in 5 ml. EtOH and 0.5 ml. Et3N is refluxed 4 hrs. to give 60% 3-isobutyl-4-phenyl-4-hydroxyoxazolidin-2-one, m. 120-3.degree. (C6H6-ligroine). Similarly prepd. are the folowing III (R and m.p. given): Me, 146-8.degree. (EtOH); Et, 104-5.degree. (EtOH); iso-Pr, 154-6.degree. (C6H6-ligroine); allyl, 110-11.degree. (EtOH-water); cyclopropyl, 140-2.degree. (C6H6-ligroine). A soln. of 2 g. I in 15 ml. HOAc is refluxed 8 hrs. to give 94% 4-phenyl-3-methyl-4-oxazolin-2-one, m. 85-6.degree. (C6H6-ligroine). Similarly prepd. are the following IV (R, m.p., and % yield given): iso-Pr, 83-4.degree. (ligroine), 81; iso-Bu, -, -; tert-Bu, 122-3.degree. (EtOH), 10.8; allyl, 43-6.degree. (EtOH-water), 50; cyclopropyl, 65-6.degree. (EtOH-water), 52; cyclopentyl, 112-13.degree. (EtOH), 60; cyclohexyl, 99-100.degree. (C6H6-ligroine), 70; p-MeOC6H4, 135-6.degree. (EtOH), 85. A soln. of 6.12 g. BzCH2OH in 80 ml. C6H6 and 10 ml. pyridine is treated at 0.degree. with 25 ml. 20% COCl2(PhMe) and the mixt. is agitated 1 hr. at 0.degree. to give 50% bis(phenacyl) carbonate, m. 116-16.5.degree. (C6H6). IV (R = cyclohexyl) shows antidepressant activity in mice at 300 mg./kg.; III (R = tert-Bu) and IV (R = iso-Pr) demonstrate fungicidal activity.
IT **13098-02-7P 13098-04-9P 13098-05-0P**
13626-63-6P 13626-64-7P 13626-67-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
RN 13098-02-7 HCAPLUS
CN Carbamic acid, (1,1-dimethylethyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)

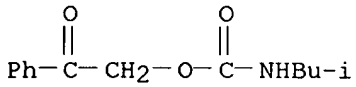


RN 13098-04-9 HCAPLUS
CN Ethanone, 2-[[(methylamino)carbonyl]oxy]-1-phenyl- (9CI) (CA INDEX NAME)

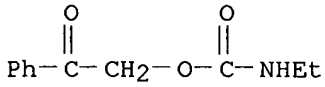




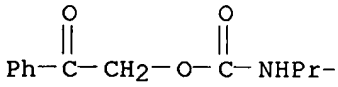
RN 13098-05-0 HCAPLUS
CN Carbamic acid, (2-methylpropyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)



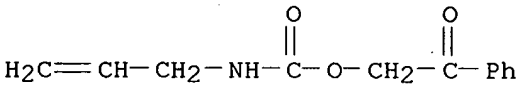
RN 13626-63-6 HCAPLUS
CN Carbamic acid, ethyl-, ester with 2-hydroxyacetophenone (8CI) (CA INDEX NAME)



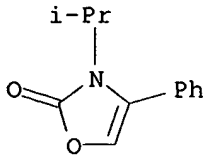
RN 13626-64-7 HCAPLUS
CN Carbamic acid, (1-methylethyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)



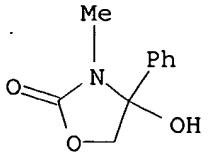
RN 13626-67-0 HCAPLUS
CN Carbamic acid, allyl-, ester with 2-hydroxyacetophenone (8CI) (CA INDEX NAME)



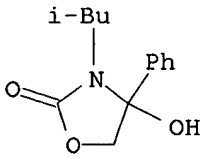
IT **13098-03-8P 13098-06-1P 13098-07-2P**
13626-72-7P 13626-73-8P 13626-74-9P
13626-76-1P 13626-78-3P 13626-79-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 13098-03-8 HCAPLUS
CN 2(3H)-Oxazolone, 3-(1-methylethyl)-4-phenyl- (9CI) (CA INDEX NAME)



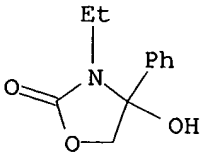
RN 13098-06-1 HCAPLUS
CN 2-Oxazolidinone, 4-hydroxy-3-methyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



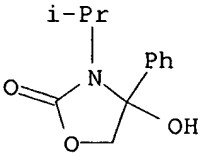
RN 13098-07-2 HCAPLUS
CN 2-Oxazolidinone, 4-hydroxy-3-(2-methylpropyl)-4-phenyl- (9CI) (CA INDEX NAME)



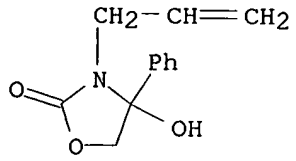
RN 13626-72-7 HCAPLUS
CN 2-Oxazolidinone, 3-ethyl-4-hydroxy-4-phenyl- (8CI) (CA INDEX NAME)



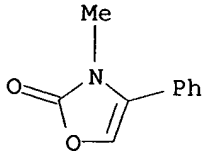
RN 13626-73-8 HCAPLUS
CN 2-Oxazolidinone, 4-hydroxy-3-isopropyl-4-phenyl- (8CI) (CA INDEX NAME)



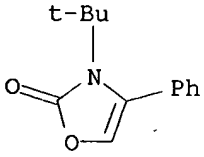
RN 13626-74-9 HCAPLUS
CN 2-Oxazolidinone, 3-allyl-4-hydroxy-4-phenyl- (8CI) (CA INDEX NAME)



RN 13626-76-1 HCAPLUS
CN 4-Oxazolin-2-one, 3-methyl-4-phenyl- (8CI) (CA INDEX NAME)



RN 13626-78-3 HCAPLUS
CN 4-Oxazolin-2-one, 3-tert-butyl-4-phenyl- (8CI) (CA INDEX NAME)



RN 13626-79-4 HCAPLUS
CN 4-Oxazolin-2-one, 3-allyl-4-phenyl- (8CI) (CA INDEX NAME)